

Down to the metal with scikit-learn

Andreas Müller Columbia University, scikit-learn







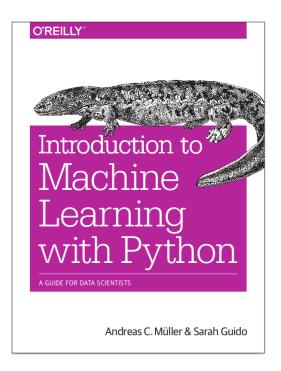






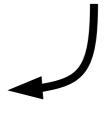




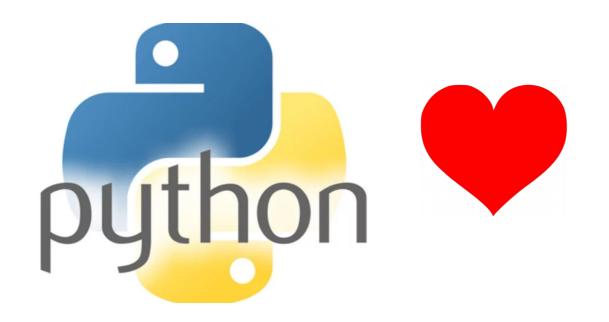


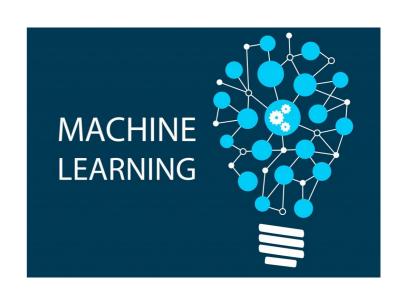






What is scikit-learn?





Classification Regression Clustering Semi-Supervised Learning Feature Selection **Feature Extraction** Manifold Learning **Dimensionality Reduction** Kernel Approximation Hyperparameter Optimization **Evaluation Metrics** Out-of-core learning





















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Virgile Fritsch VirgileFritsch



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Wei Li



Mission

Commoditize and Democratize Machine Learning

Basic API

Representing Data

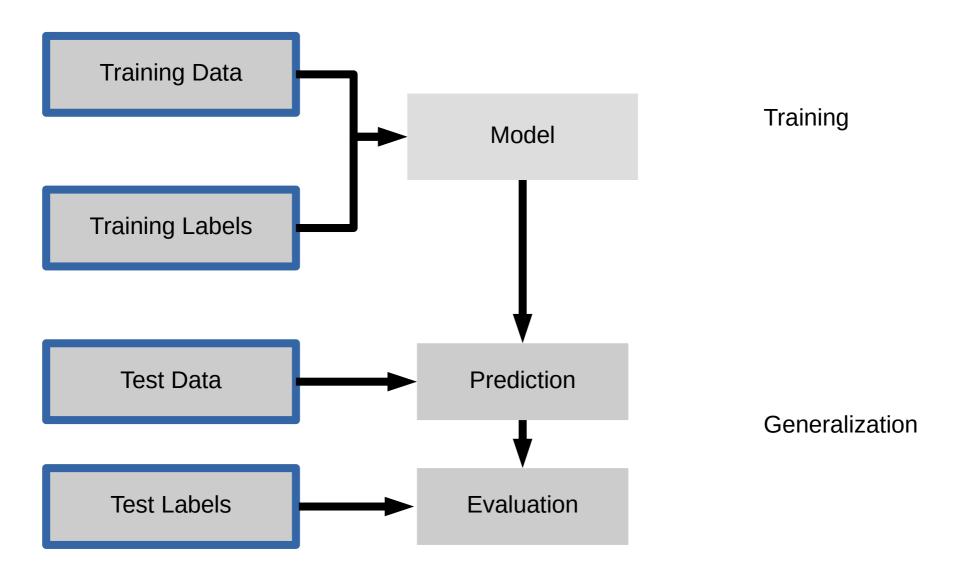


1.1	2.2	3.4	5.6	1.0	\setminus
6.7	0.5	0.4	2.6	1.6	_
2.4	9.3	7.3	6.4	2.8	
1.5	0.0	4.3	8.3	3.4	
0.5	3.5	8.1	3.6	4.6	
5.1	9.7	3.5	7.9	5.1	
3.7	7.8	2.6	3.2	6.3	
	6.7 2.4 1.5 0.5 5.1	 6.7 0.5 2.4 9.3 1.5 0.0 0.5 3.5 5.1 9.7 	6.70.50.42.49.37.31.50.04.30.53.58.15.19.73.5	6.7 0.5 0.4 2.6 2.4 9.3 7.3 6.4 1.5 0.0 4.3 8.3 0.5 3.5 8.1 3.6 5.1 9.7 3.5 7.9	2.4 9.3 7.3 6.4 2.8 1.5 0.0 4.3 8.3 3.4 0.5 3.5 8.1 3.6 4.6 5.1 9.7 3.5 7.9 5.1

one feature

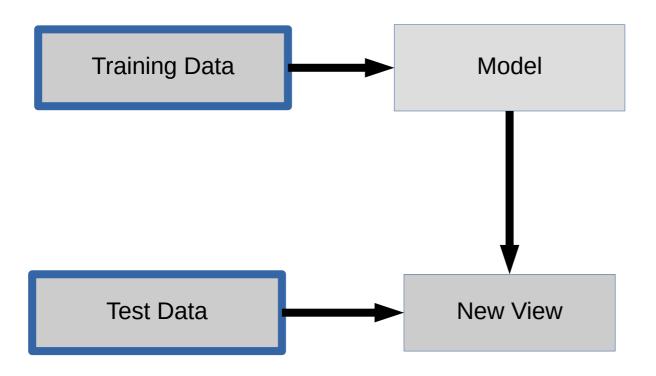
outputs / labels

Supervised Machine Learning



clf = RandomForestClassifier() clf.fit(X_train, y_train) Training Data Model Training Labels y_pred = clf.predict(X_test) **Test Data** Prediction clf.score(X_test, y_test) **Test Labels Evaluation**

Unsupervised Machine Learning



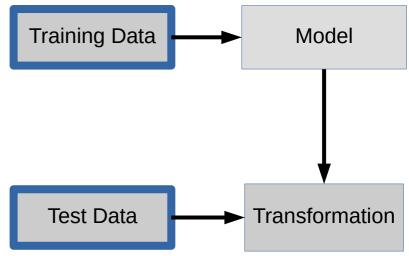
Unsupervised Transformations

```
pca = PCA()

pca.fit(X_train)

Training Data

X_new = pca.transform(X_test)
```



Core API Summary

estimator.fit(X, [y])

estimator.predict

estimator.transform

Classification

Preprocessing

Regression

Dimensionality reduction

Clustering

Feature selection

Feature extraction

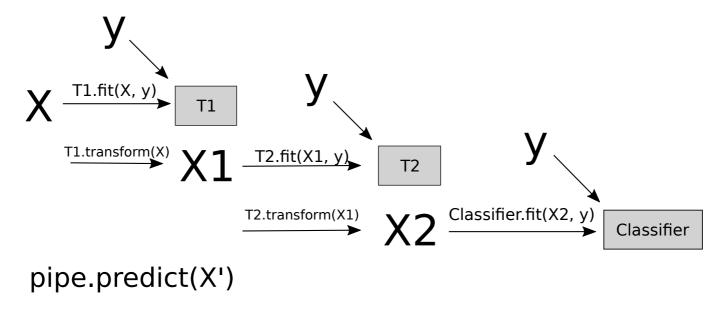
Cross -Validated Grid Search

Pipelines

pipe = make_pipeline(T1(), T2(), Classifier())

T1 T2 Classifier

pipe.fit(X, y)



$$X^{\mathsf{T1.transform}(X')} X^{\mathsf{T1}} \xrightarrow{\mathsf{T2.transform}(X'1)} X^{\mathsf{T2}} \xrightarrow{\mathsf{Classifier.predict}(X'2)} Y^{\mathsf{T3}}$$

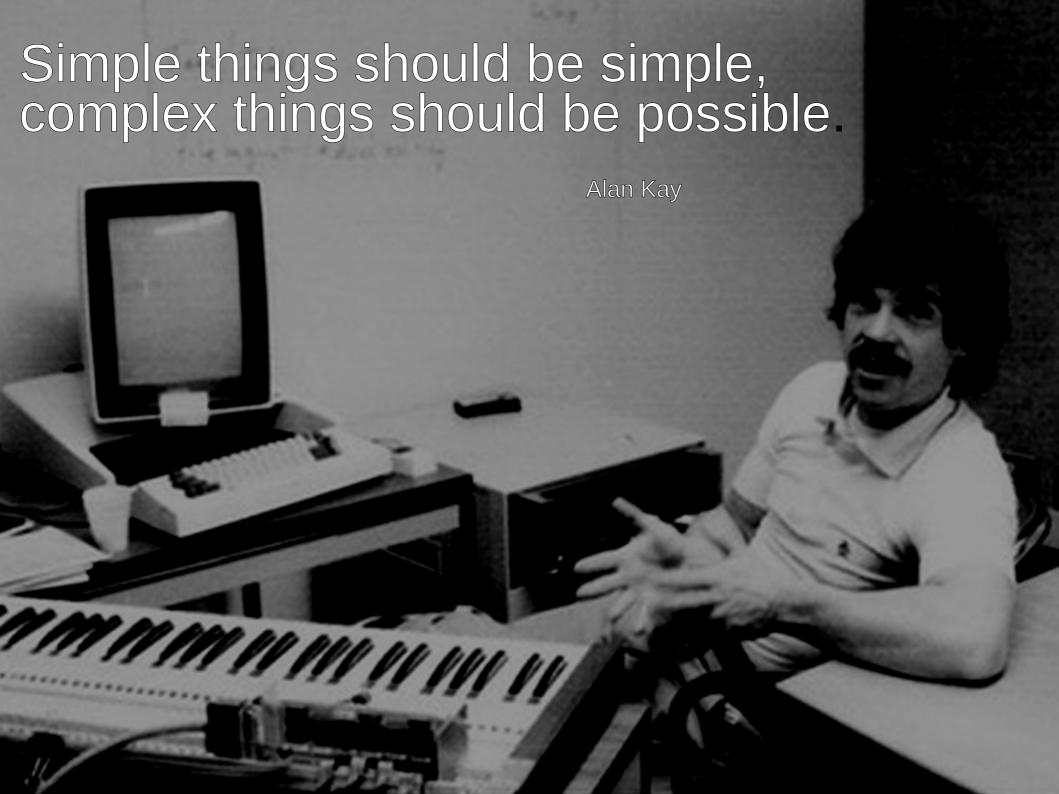
Pipelines

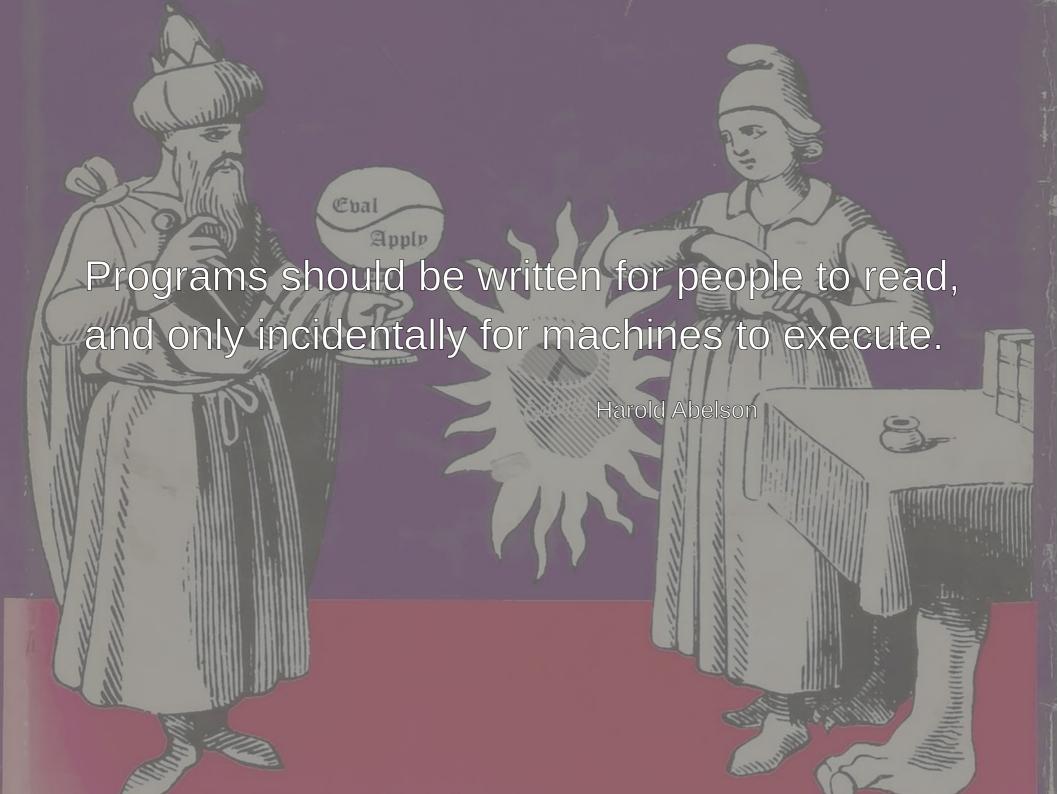
```
from sklearn.pipeline import make_pipeline
pipe = make_pipeline(StandardScaler(), SVC())
pipe.fit(X_train, y_train)
pipe.predict(X_test)
```

Guiding Ideas

Goals:

Maintainability Ease of use





Simplicity

```
lr = LogisticRegression()
lr.fit(X_train, y_train)
lr.score(X_test, y_test)
```

Consistency

```
grid = GridSearchCV(svm,param_grid)
grid.fit(X_train, y_train)
grid.score(X_test, y_test)
```

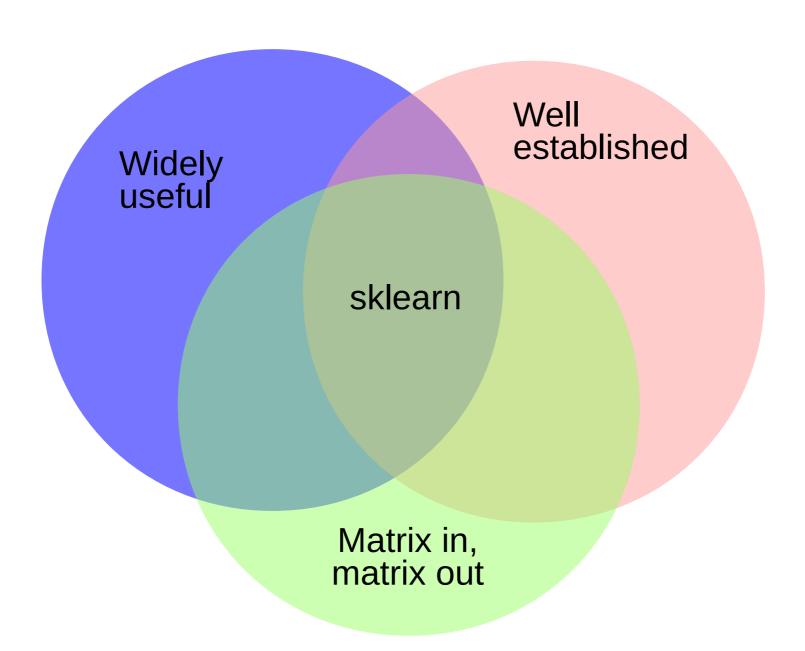
Composition

Default Parameters

Flat Class Hierarchy, Few Types

- Numpy arrays / sparse matrices
- Estimators
- Cross-validation objects
- Scorers

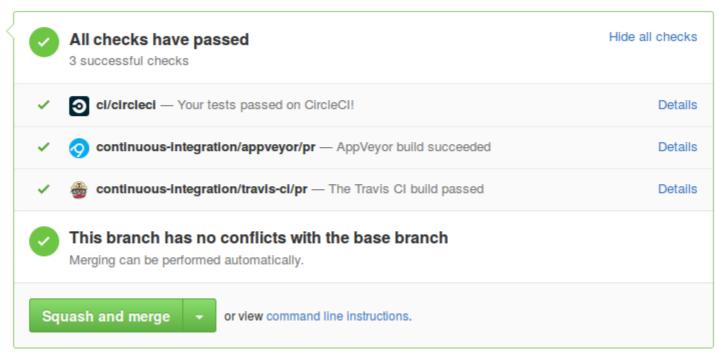
Scoping



Testing & Continuous Integration

Add more commits by pushing to the more_repr branch on amueller/scikit-learn.





Three way documentation

1.9. Ensemble methods

The goal of **ensemble methods** is to combine the predictions of several base estimators built with a given learning algorithm in order to improve generalizability / robustness over a single estimator.

Two families of ensemble methods are usually distinguished:

 In averaging methods, the driving principle is to build several estimators independently and then to average their predictions. On average, the combined estimator is usually better than any of the single base estimator because its variance is reduced.

Examples: Bagging methods, Forests of randomized trees, ...

 By contrast, in boosting methods, base estimators are built sequentially and one tries to reduce the bias of the combined estimator. The motivation is to combine several weak models to produce a powerful ensemble.

Examples: AdaBoost, Gradient Tree Boosting, ...

sklearn.ensemble.RandomForestClassifier

class sklearn.ensemble. RandomForestClassifier (n_estimators=10, criterion='gini', max_depth=None, min_samples_split=2, min_samples_leaf=1, min_weight_fraction_leaf=0.0, max_features='auto', max_leaf_nodes=None, bootstrap=True, oob_score=False, n_jobs=1, random_state=None, verbose=0, warm_start=False) [source]

A random forest classifier.

A random forest is a meta estimator that fits a number of decision tree classifiers on various sub-samples of the dataset and use averaging to improve the predictive accuracy and control over-fitting.

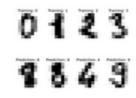
Parameters: n estimators: integer, optional (default=10)

The number of trees in the forest.

criterion: string, optional (default="gini")

The function to measure the quality of a split. Supported criteria are "gini" for the Gini impurity and "entropy" for the information gain. Note: this parameter is tree-specific.

Examples



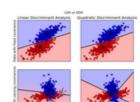
Recognizing hand-written digits



Plot classification probability



Classifier comparison



Linear and Quadratic
Discriminant Analysis

with confidence ellipsoid

Behind the scenes

API implementation & contracts

Method Chaining

Fit must return self:

fit resets

```
from sklearn.tree import DecisionTreeClassifier
tree = DecisionTreeClassifier(max_depth=10)
tree.fit(iris.data, iris.target)
score_iris = tree.score(iris.data, iris.target)
tree.fit(digits.data, digits.target)
score_digits = tree.score(digits.data, digits.target)
```

__init__ does nothing

get_params & set_params

```
def get_params(self, deep=True):
    out = dict()
    for key in signature(self.__init__):
        value = getattr(self, key, None)
        if deep and hasattr(value, 'get_params'):
            deep_items = value.get_params().items()
            out.update((key + '__' + k, val) for k, val in deep_items)
        out[key] = value
    return out
```

Used in GridSearchCV etc.

Not __init__ !!!

All parameter validation etc in fit!

(only) fit mutates self

- __init__ only remembers construction parameters
- Transform / score etc don't change object
- Fit returns self but mutates object!

Estimated attributes

```
Attributes
 components : array, shape (n components, n features)
     Principal axes in feature space, representing the directions of
     maximum variance in the data. The components are sorted by
     ``explained variance ``.
 explained variance : array, shape (n components,)
     The amount of variance explained by each of the selected components.
     Equal to n components largest eigenvalues
     of the covariance matrix of X.
     .. versionadded:: 0.18
 explained variance ratio : array, shape (n components,)
     Percentage of variance explained by each of the selected components.
     If ``n components`` is not set then all components are stored and the
     sum of the ratios is equal to 1.0.
 singular values : array, shape (n components,)
     The singular values corresponding to each of the selected components.
     The singular values are equal to the 2-norms of the ``n components``
     variables in the lower-dimensional space.
Leaves two kinds of attributes:
arguments to init; things estimated during fit
```

fit_transform / fit_predict

In general: computational shortcut:

```
pca = PCA()
pca.fit(X)
X_pca = pca.transform(X)
X_pca2 = pca.fit_transform(X)
```

Clustering / Manifold learning: Not inductive.

```
tsne = TSNE()
X_tsne = tsne.fit_transform(X)
```

```
dbscan = DBSCAN()
cluster_labels = dbscan.fit_predict(X)
```

check_estimator

```
class TemplateClassifier(BaseEstimator, ClassifierMixin):
   def init (self, demo param='demo'):
        self.demo param = demo param
   def fit(self, X, y):
       # Check that X and y have correct shape
       X, y = \text{check } X y(X, y)
       # Store the classes seen during fit
       self.classes = unique labels(y)
        self.X = X
        self.v = v
       # Return the classifier
        return self
   def predict(self, X):
        closest = np.argmin(euclidean distances(X, self.X), axis=1)
        return self.v [closest]
```

check_estimator(TemplateClassifier)

AssertionError: Error message does not include the expected string: 'fit'. Observed error message: "'TemplateClassifier' object has no attribute 'X_'"

Other API Building Blocks

Scorers

Cross-validation iterators

```
grid = GridSearchCV(SVC(), param_grid, cv=5)
cv = KFold(n_split=5, shuffle=True, random_state=3)
grid = GridSearchCV(SVC(), param_grid, cv=cv)
```

```
cv = RepeatedKFold(n_split=5, n_repeats=10)
grid = GridSearchCV(SVC(), param_grid, cv=cv)
```

CV Iterators API

```
def split(self, X, y=None, groups=None):
     """Generate indices to split data into training and test set.
     Parameters
    X : array-like, shape (n samples, n features)
        Training data, where n samples is the number of samples
         and n features is the number of features.
     y : array-like, of length n samples
         The target variable for supervised learning problems.
     groups : array-like, with shape (n samples,), optional
        Group labels for the samples used while splitting the dataset into
         train/test set.
     Returns
    train : ndarray
        The training set indices for that split.
     test : ndarray
         The testing set indices for that split.
kfold = KFold(n_splits=5)
for train, test in kfold.split(X, y):
    X_train = X[train]
    X_test = X[test]
```

Misc functions

- Scoring functions func(y_true, y_pred/y_scores, ...)
- Pairwise Distances/kernels euclidean_distances rbf_kernel
- Evaluation: cross_validate learning_curve roc_curve
- Helpers: train_test_split

Development Practices

Standards for OSS

Everything discussed in the open. Every convention and process documented.

Development guide

http://scikit-learn.org/dev/developers/contributing.

Contains:

- API details
- Bug report guidelines
- PR guidelines
- Reviewing guidelines
- How to find issues
- Details of CI

Sphinx / numpydoc

```
class MultinomialNB(BaseDiscreteNB):
    Naive Bayes classifier for multinomial models
    The multinomial Naive Bayes classifier is suitable for classification with
   discrete features (e.g., word counts for text classification). The multinomial distribution normally requires integer feature counts. However,
    in practice, fractional counts such as tf-idf may also work.
    Read more in the :ref: 'User Guide <multinomial_naive_bayes>'.
    Parameters
    alpha: float, optional (default=1.0)
        Additive (Laplace/Lidstone) smoothing parameter
        (0 for no smoothing).
    fit_prior : boolean, optional (default=True)
        Whether to learn class prior probabilities or not.
        If false, a uniform prior will be used.
    class prior : array-like, size (n classes,), optional (default=None)
        Prior probabilities of the classes. If specified the priors are not
        adjusted according to the data.
    class_log_prior_ : array, shape (n_classes, )
        Smoothed empirical log probability for each class.
   intercept_ : property
    Mirrors ``class_log_prior_`` for interpreting MultinomialNB
        as a linear model.
    feature_log_prob_ : array, shape (n_classes, n_features)
    Empirical log probability of features
        given a class, ``P(x_i|y)``
   coef_ : property
   Mirrors ``feature_log_prob_`` for interpreting MultinomialNB
        as a linear model.
    class count : array, shape (n classes,)
        Number of samples encountered for each class during fitting. This
        value is weighted by the sample weight when provided.
    feature_count_ : array, shape (n_classes, n_features)
        Number of samples encountered for each (class, feature)
        during fitting. This value is weighted by the sample weight when
        provided.
    Examples
    >>> import numpy as np
    >>> X = np.random.randint(5, size=(6, 100))
    >>> y = np.array([1, 2, 3, 4, 5, 6])
    >>> from sklearn.naive_bayes import MultinomialNB
    >>> clf = MultinomialNB()
    >>> clf.fit(X, y)
    MultinomialNB(alpha=1.0, class prior=None, fit prior=True)
    >>> print(clf.predict(X[2:3]))
    [3]
    Notes
   For the rationale behind the names `coef ` and `intercept `, i.e. naive Bayes as a linear classifier, see J. Rennie et al. (2003),
    Tackling the poor assumptions of naive Bayes text classifiers, ICML.
    References
    C.D. Manning, P. Raghavan and H. Schuetze (2008). Introduction to
    Information Retrieval. Cambridge University Press, pp. 234-265.
    http://nlp.stanford.edu/IR-book/html/htmledition/naive-bayes-text-classification-1.html
```

sklearn.naive bayes.MultinomialNB

class sklearn.naive bayes. MultinomialNB (alpha=1.0, fit prior=True, class prior=None) Naive Bayes classifier for multinomial models The multinomial Naive Bayes classifier is suitable for classification with discrete features (e.g., word counts for text classification). The multinomial distribution normally requires integer feature counts. However, in practice, fractional counts such as tf-ldf may also work Read more in the User Guide Parameters: alpha: float, optional (default=1.0) Additive (Laplace/Lidstone) smoothing parameter (0 for no smoothing) fit_prior : boolean, optional (default=True) Whether to learn class prior probabilities or not. If false, a uniform prior will be used. class prior : array-like, size (n classes.), optional (default=None) Prior probabilities of the classes. If specified the priors are not adjusted according to the data. Attributes: class log prior : array, shape (n classes,) Smoothed empirical log probability for each class. intercept_: array, shape (n_classes,) Mirrors class_log_prior_ for Interpreting MultinomialNB as a linear model. feature_log_prob_: array, shape (n_classes, n_features) Empirical log probability of features given a class, P(x i|v) coef_: array, shape (n_classes, n_features) Mirrors feature_log_prob_ for interpreting MultinomialNB as a linear model. class count : array, shape (n classes.) Number of samples encountered for each class during fitting. This value is weighted by the sample weight when provided. feature count : array, shape (n classes, n features) Number of samples encountered for each (class, feature) during fitting. This value is weighted by the sample weight when provided.

Notes

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References

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Examples

```
>>> import numpy as np
>>> X = np.random.randint(5, size=(6, 100))
>>> y = np.array([1, 2, 3, 4, 5, 0])
>>> from sklearn.naive_bayes_import MultinomialNB
>>> cirf = MultinomialNB()
>>> cirf.fit(X, y)
MultinomialNB(alpha=1.0, class_prior=None, fit_prior=True)
>>> print(cif.predict(X[2:3]))
[3]
```

Methods

Fit Naive Bayes classifier according to X, y
Get parameters for this estimator.
Incremental fit on a batch of samples.
Perform classification on an array of test vectors X.
Return log-probability estimates for the test vector X.
Return probability estimates for the test vector X.
Returns the mean accuracy on the given test data and labels.
Set the parameters of this estimator.

Sphinx / numpydoc

.. svm:

Support Vector Machines

.. currentmodule:: sklearn.svm

Support vector machines (SVMs) are a set of supervised learning methods used for :ref:`classification <svm_classification>`, :ref:`regression <svm_regression>` and :ref:`outliers detection <svm_outlier_detection>`.

The advantages of support vector machines are:

- Effective in high dimensional spaces.
- Still effective in cases where number of dimensions is greater than the number of samples.
- Uses a subset of training points in the decision function (called support vectors), so it is also memory efficient.
- Versatile: different :ref:`svm_kernels` can be specified for the decision function. Common kernels are provided, but it is also possible to specify custom kernels.

The disadvantages of support vector machines include:

- If the number of features is much greater than the number of samples, the method is likely to give poor performances.
- SVMs do not directly provide probability estimates, these are calculated using an expensive five-fold cross-validation (see :ref:`Scores and probabilities <scores_probabilities>`, below).

The support vector machines in scikit-learn support both dense (``numpy.ndarray`` and convertible to that by `numpy.asarray``) and sparse (any ``scipy.sparse``) sample vectors as input. However, to use an SVM to make predictions for sparse data, it must have been fit on such data. For optimal performance, use C-ordered ``numpy.ndarray`` (dense) or ``scipy.sparse.csr_matrix`` (sparse) with ``dtype=float64``.



1.4. Support Vector Machines

- 1.4.1. Classification
- 1.4.1.1. Multi-class classification
- 1.4.1.2. Scores and probabilities
- 1.4.1.3. Unbalanced problems
- 1.4.2. Regression
- 1.4.3. Density estimation, novelty detection
- 1.4.4. Complexity
- 1.4.5. Tips on Practical Use
- 1.4.6. Kernel functions
- 1.4.6.1. Custom Kernels
- 1.4.6.1.1. Using Python functions as kernels
- 1.4.6.1.2. Using the Gram matrix
- 1.4.6.1.3. Parameters of the RBF Kernel
- 1.4.7. Mathematical formulation

1.4. Support Vector Machines

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Search ×

Support vector machines (SVMs) are a set of supervised learning methods used for classification, regression and outliers detection

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- Still effective in cases where number of dimensions is greater than the number of samples.
- Uses a subset of training points in the decision function (called support vectors), so it is also memory
 efficient
- Versatile: different Kernel functions can be specified for the decision function. Common kernels are
 provided, but it is also possible to specify custom kernels.

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Deprecations / backward compatibility

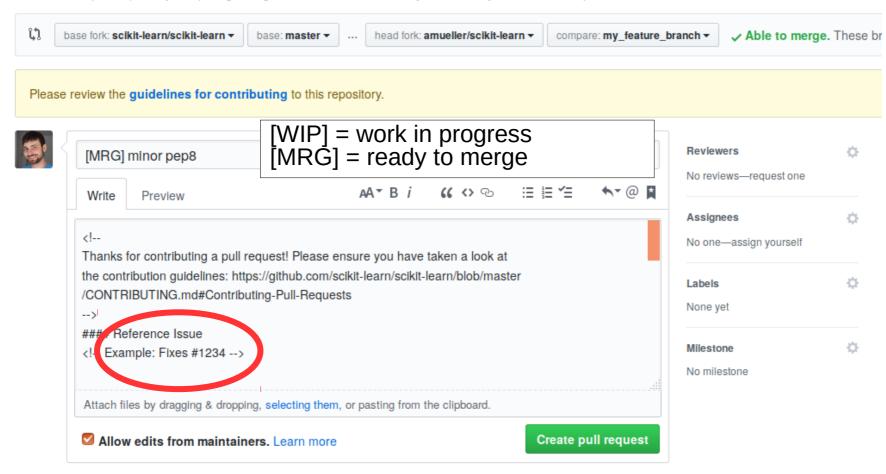
Don't change any behavior (except bug fixes)

Practical Notes on Contributing

Describing PR

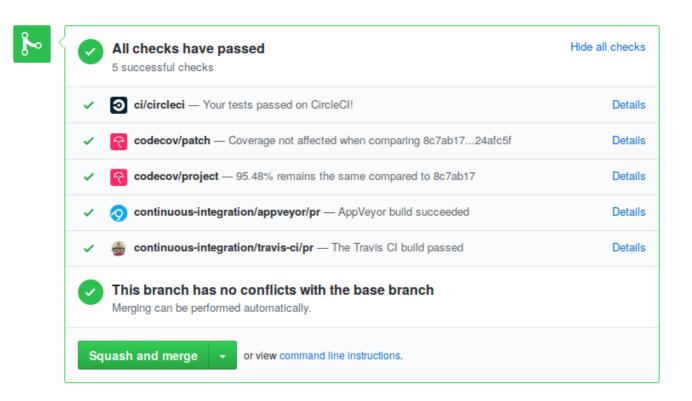
Open a pull request

Create a new pull request by comparing changes across two branches. If you need to, you can also compare across forks.



Regression tests

- Are mandatory! For everything (except documentation changes)!
- Make sure continuous integration passes:



What's next?

- Wait for reviews (be patient).
- Address review comments in the same branch.
- Pushing to your fork will update the PR
- Reviewers will "approve" PR or change title to [MRG + 1]
- You need two approvals for a merge.

Finding Issues

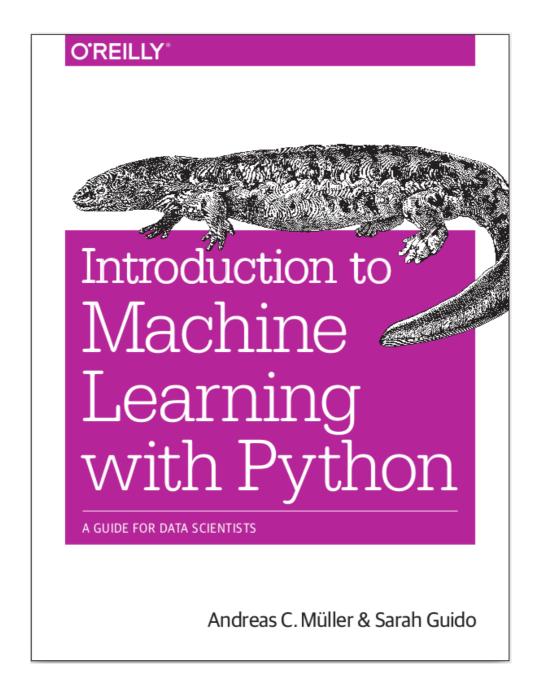
- Check "need contributor", "easy" and "sprint" issues.
- Something unclear in the docs? Fix it!
- Can't fix something that's unclear? Open an issue!
- Problem that you keep running into: Open an issue!
- Find stalled PRs (the author didn't address reviews for ~>1 month) and continue them!

Reviewing

- You can review PRs and issues!
- Some bugs are not confirmed. See if you can confirm them and under what conditions?
- You can review documentation PRs for language and whether they are clear to you.
- You can review code changes on whether they address the issue (might be a bit tricky).
- Don't be afraid to ask clarifying questions!

Final words

- Pick something TRIVIALLY SIMPLE as the first contribution.
- You can do the cool stuff afterwards!
- There might be interesting issues that are not appropriately tagged.
- Consider finishing up stalled PRs



Thank you.



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